2022 DOE Vehicle Technologies Office
Annual Merit Review

Independent Fuel Property Effects of Fuel Volatility on Low Temperature Heat Release and Fuel Autoignition

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2. Oak Ridge National Laboratory, presenter
3. Argonne National Laboratory

Project ID # ace177

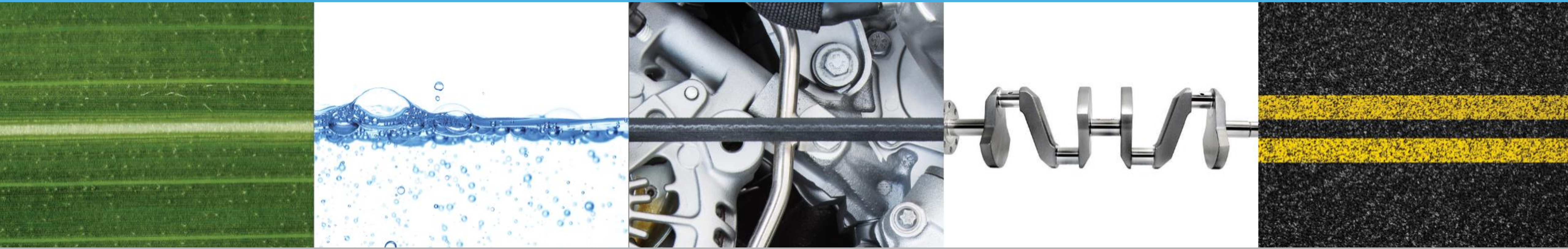
June 22, 2022

CO-OPTIMIZATION OF FUELS & ENGINES

better fuels | better vehicles | sooner

Oak Ridge National Laboratory

Argonne National Laboratory



Overview

Timeline

- Project awards announced 5/10/21
- CRADA finalized on 4/8/22
- 18-month duration
  - Complete 10/8/23

Budget

- Total CRADA value: $315,000
  - DOE funds to ORNL: $140,000
  - DOE funds to ANL: $110,000
  - Shell funds to ANL: $30,000
  - Shell in-kind funds: $35,000

Any proposed future work is subject to change based on funding level

Barriers

- Incomplete understanding of fuel property effects on engine performance
  - High fuel volatility (vapor pressure) suppresses suppress low temperature heat release
  - Project developing knowledge and computational tools
- Better knowledge needed for decarbonization transition

CRADA Partners

- Shell Global Solutions
  - PI, custom fuel blends
- Oak Ridge National Laboratory
  - Experimental engine facility
- Argonne National Laboratory
  - Computation Simulations

RELEVANCE

Improved Predictive Tools are Needed to Optimize for Properties of Sustainable Fuels

Overall Co-Optima Goal

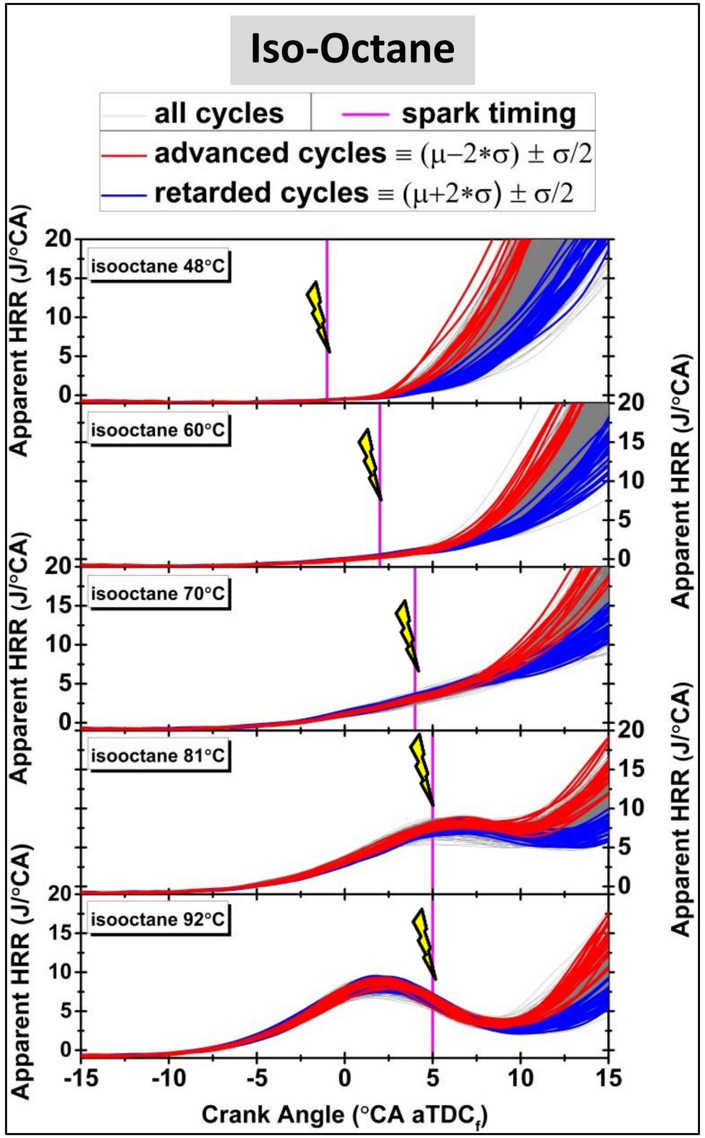
better fuels | better vehicles | faster

Central Fuel Property Hypothesis

Equivalent fuel properties will result in equivalence performance, regardless of the composition

This Project will Close a Fuel Property-Performance Gap

- Shell identified that fuels with high volatility (vapor pressure) suppress low-temperature heat release (LTHR)
- Phenomenon is independent of research and motor octane number (RON and MON)
    - Important for boosted SI engines
    - Important to heavy-duty advanced compression ignition (ACI) strategies
- Knowledge gained applies to low lifecycle carbon fuels (LLCFs)



Szybist and Splitter,
DOI: 10.1016/j.combustflame.2016.12.002

APPROACH

Experimental and Computational Effort to Test Hypothesis that Cause is Preferential Evaporation

Hypothesis: Preferential evaporation of fuels can create compositional and reactivity stratification

- Most volatile components contributing to high vapor pressure tend to have high octane number
- The most volatile components dominate reactivity when the system is stratified, resulting in less LTHR
- Composition of most volatile components change with LLCFs, including due to azeotropic behavior

Project uses capabilities and expertise developed during the Co-Optima Initiative

Shell: Custom Fuel Blends with Sustainable Co-Optima Blendstocks

[illegible] Low Volatility (LV) Fuels

[illegible]	[illegible]	F7a	F8a	F14a	F15a	F16a	F17a	F18a	F19a
[illegible]	[illegible]	9	10	≤10	≤10	≤10	≤10	≤10	≤10
M124049 (an aromatic) [V%]	0	20	10	10	10	10	10	10	10
Ethanol [V%]	0	0	10	0	0	0	0	0	0
Isopropanol [V%]	0	0	0	0	0	0	10	0	0
Prenol [V%]	0	0	0	0	10	0	0	0	0
Di-isobutylene [V%]	0	0	0	0	0	0	0	0	10
Cyclopentane [V%]	0	0	0	0	0	10	0	0	0
M126642 [V%]	0	0	0	5	0	0	0	10	0
Mxxxxxx	0	0	0	100 ppm	0	0	0	100 ppm	0

Baseline fuel F6a is an E10 Regular gasoline. F6a, F7a, and F8a are reblends of prior test fuels. F14a-F19a are new experimental blends.

Fuels F7a, F8a, etc., prepared by splash blending components (M124049, ethanol, isopropanol, etc.) on top of fuel F6a

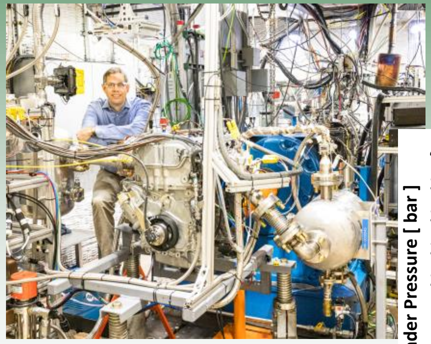
Shell High Volatility (HV) Fuels

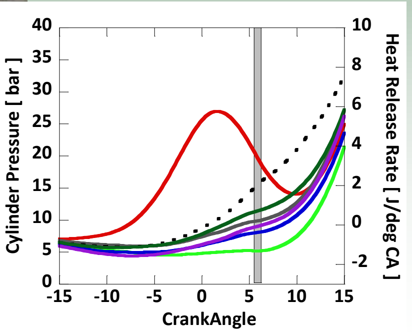
Property/Component	F6b	F7b	F8b	F14b	F15B	F16B	F17b	F18b	F19b
ASVP (psi)	13	11	12	12	12	12	12	12	12
Light ends (butanes/butenes) [V%]	tbd	--	--	--	--	--	--	--	--

HV fuels prepared by splash blending light ends on top of the respective LV fuel. Same V% used for each.

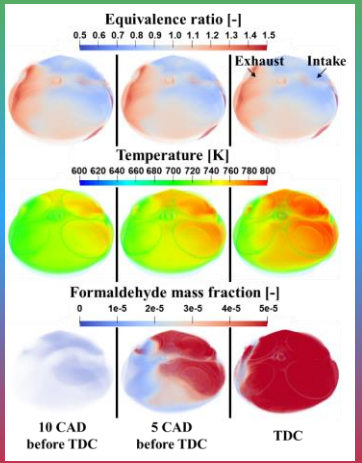
The V% of light ends is determined by adding enough to F6a to increase ASVP 2 psi. Whatever that is, add the same to each LV fuel.

ORNL: Experimental Engine Capabilities to Directly Measure LTHR





ANL: Computational Simulations of ORNL Engine



Project Tasks and Timeline

Task No.	Task Name	Project Months																		Responsible Party
		Year 1												Year 2						
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	Design of Fuel Matrix and Blending																			Shell
2.1	Stoichiometric LTHR Measurements																			ORNL
2.2	Fuel Lean LTHR Measurements																			ORNL
3.1	A priori LTHR Simulations																			ANL
3.2	Simulations of experimental data																			ANL
4	Data Co-Analysis with NLs																			Shell
5	Reporting																			Shell

Project Status

Any proposed future work is subject to change based on funding level

Fuel Matrix Focusing on LLCF Blends Complete, Blending Underway at

- Includes Co-Optima-identified LLCF blends: ethanol, isopropanol, prenol, and di-isobutylene
- Azeotropic vapor pressure behavior well-known for some LLCFs
- Fuels blended at two different vapor pressure levels

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Prenol [V%]	0	0	0	0	10	0	0	0	0
Di-isobutylene [V%]	0	0	0	0	0	0	0	0	10
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Project Team of Shell, ORNL, and ANL. Aligned Effort to Understand LTHR Phenomenon

- Closely coordinated 18-month project utilizing capabilities developed in Co-Optima
  - Shell: Custom fuel blends using Co-Optima identified LLCFs, data analysis
  - ORNL: Experimental measurements of LTHR
  - ANL: Computational simulations
- Outcome will provide an understanding if preferential evaporation is responsible for suppression of LTHR in high volatility fuel blends

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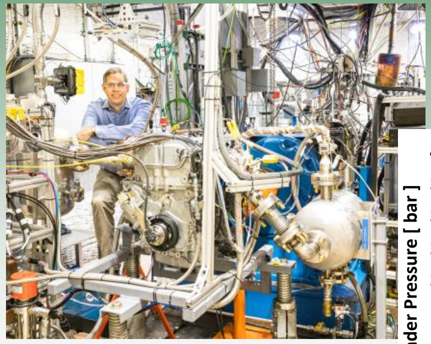

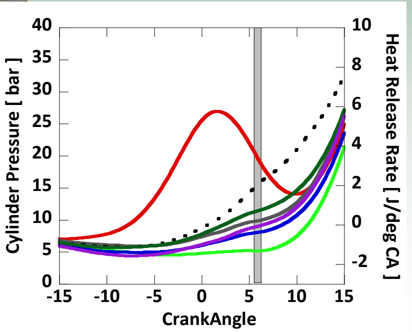

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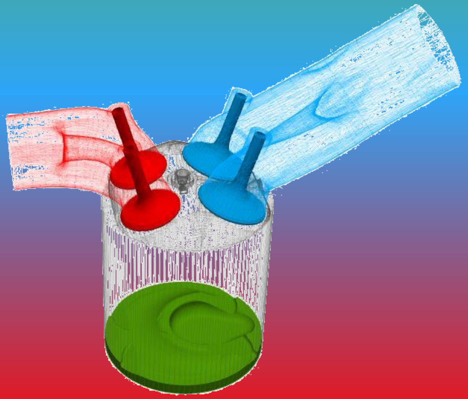

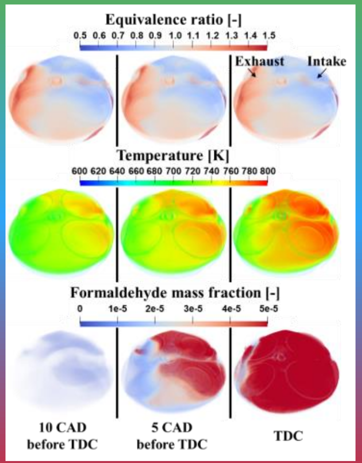

Planned Research will Achieve the Following Milestones

1	Stoichiometric Measurements of LTHR (ORNL)	November 2022
2	A priori LTHR simulations (ANL)	November 2022
3	Fuel-Lean Measurements of LTHR (ORNL)	May 2023
4	Simulations of ORNL Experimental Data (ANL)	August 2023
5	Data Analysis Complete (Shell)	September 2023
6	Final Report Submitted (Shell)	October 2023

Any proposed future work is subject to change based on funding level

SUMMARY

Relevance

- *Developing predictive tools to accelerate the adoption of sustainable fuels. better fuels | better vehicles | faster*
- *Volatile fuels (high vapor pressure) have been observed to suppress LTHR more than properties predict*
- *Composition high vapor pressure can change with sustainable low lifecycle carbon fuels*
- *This investigation will test the hypothesis that it is due to preferential evaporation creating reactivity stratification*

Approach Combines Design of Custom Fuels, Engine Experiments, and Computational Simulation

- *Custom fuel blends of sustainable, low lifecycle carbon fuels identified from Co-Optima*
- *Unique engine experiments developed for Co-Optima using late combustion phasing to temporally separate LTHR from deflagration (stoichiometric experiments relevant to boosted spark ignition, fuel-lean experiments relevant to advanced compression ignition for heavy-duty and offroad)*
- *Unique simulation approach developed for Co-Optima to accurately capture LTHR magnitude with different fuels*

Accomplishments: Project in Early Stages

- *CRADA fully-executed in April 2022*
- *Designed fuel matrix with target fuel compositions and properties*
- *Fuels currently being blended at Shell facility*

Collaborations

- *Team of Shell, ORNL, and ANL*
- *Aligned project tasks to share data to test project hypothesis*

Future Work

- *Experimental measurements of LTHR in engine using Shell custom fuel blends*
- *Simulation of ORNL data by ANL*
- *All tasks are well-defined and aligned*

Any proposed future work is subject to change based on funding level